Uncertainty in Thermophysical Property Data and Correlations: How Does it Affect Process Simulation? (Invited)

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In any process simulation, the process design engineer makes several choices that affect the uncertainty of the final design or performance prediction. Without an adequate characterization of this uncertainty, the risk of over-design or under-design is essentially unknown. The inverse problem of determining the value of more or better data or correlations similarly requires an uncertainty analysis.

Through case studies, we present techniques for analyzing design uncertainty as it is affected by errors in experimental data (both random and systematic), models, model parameters, and process simulators. As we build and choose models, obtain and report experiment data, regress parameters, and set up the computer process simulations, we need always to have an estimate of the uncertainty. Seemingly small errors in any step can lead to large uncertainties in the final design—and these uncertainties are often completely hidden.

New Monte Carlo techniques for uncertainty analyses can provide estimates of the effects of systematic as well as random error, especially when the data or the model parameters are highly correlated. Other novel techniques for regression of correlated parameters in nonlinear models can provide significantly improved correlations as well as better uncertainty estimates. Future directions for closing the loop of data-model-regression-simulation-data will be presented.